

Dynamics and Control of Distillation using *Aspen*

Bachelor in Technology
In
Chemical Engineering

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CERTIFICATE

This is to certify that the report entitled, '**Dynamics and control of distillation using ASPEN**' submitted by **Vishal Kaushik (107CH039)** in partial fulfillment of the requirements for the award of Bachelor of Technology Degree in Chemical Engineering at the National Institute Of Technology, Rourkela is an authentic work carried out by them under my supervision and guidance.

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ABSTRACT

This thesis interprets about the dynamics and control study of distillation columns using Aspen. As all of us are aware, that distillation is one of the most important separation processes in the Chemical Engineering. In the present thesis, simulation studies of the distillation column are presented. Steady state simulations are being performed using Aspen Plus followed by Aspen Dynamic simulation, licensed software of Aspen Tech. In the steady state simulation we have tried to see the effect of changing the flow rate of the extracting solvent etc., which gives criterion about the optimum flow rate in the distillation column. The basic controllers are used for controlling sump level, reflux level and molar feed flow rate. Further two important strategies used for controlling the purity of distillate are: (1) controlling the tray temperature where the maximum change of temperature is observed due to reboiler heat change (2) composition controller. Tyreus –Luyben method is used to tune the proportional integrator controller (PI) for temperature and composition control. The location of temperature controlled tray is obtained by steady state gain value. The design value of integral time constant, τ_I of temperature control and composition control configurations are found as 2.54 min. and 68.54 min. respectively. Hence, response of temperature controller is faster than the composition controller, but on account of less purity. Thus results encourage to use cascade controller.

Keywords: Aspen plus, Aspen Dynamics, Steady state simulation, Cascade control, Composition, controller, Temperature controller, Integral time constant.

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CHAPTER 1

INTRODUCTION AND LITERATURE SURVEY

1. INTRODUCTION AND LITERATURE SURVEY

1.1 GENERAL: In practice, distillation may be carried out by either of two methods. The first method is based on the production of a vapour by boiling the liquid mixture to be separated and condensing the vapor without allowing any liquid to return to the still. Then, there is no reflux. The second method is based upon the return of part of the condensate to the still under such conditions that this returning liquid is brought into the intimate contact with the vapors on their way to condenser. Either of these two methods may be conducted as a continuous or as a batch process, but the study of dynamics and control of process is one of most important part of each process.

Distillation is one of the commonly used separation technique in the chemical industries [1]. The separation is based on differences in “volatilities” (tendencies to vaporize) among various chemical components. In a distillation column the more volatile, or lighter, components are removed from the top of the column, and the less volatile, or heavier, components are removed from the lower part of the column.

Further Aspen Plus makes it easy to build and run the process simulation model by providing with a comprehensive system of the online process modelling. Process simulation allows one to predict the behaviour of a process by using basic engineering relationships, such as mass and energy balances, and phase and chemical equilibrium. Process simulation enables one to run many cases, conduct ‘what if’ analysis and perform sensitivity analysis and optimisation runs. With simulation one can design better plants and increase the profitability in the existing plants. Process simulation is helpful throughout the entire life of a process, from research and development through process design to production. Efficient design of distillation equipment requires quantitative understanding of vapor liquid equilibria. In VLE phases are expressed through vapour phase fugacity coefficients and the liquid phase activity coefficients. At low or modest pressures fugacity coefficient can be estimated easily for very simple mixtures or ideal solutions, but for non-ideal mixtures, estimation of liquid phase activity coefficient is quite difficult. Experimental mixture data are required to calculate activity coefficient. The liquid phase ideality (activity coefficient $\gamma=1$) occurs only when the components are quite similar.

The benzene toluene system is a common example. Activity coefficients of both benzene and toluene are very close to unity. However if components are dissimilar, non-ideal behaviour occurs. Consider a mixture of methanol and water. Water is very polar, Methanol is very polar on the OH end of the molecule, but the methyl end is non polar. This results in some non ideality. A large part of chemical engineering design is concerned with separation operations. Many of these are diffusional operations of the phase-contacting type, and distillation, absorption, and extraction are the most common. For rational design of such separation processes, we require quantitative information on phase equilibria in multi-component mixtures. Satisfactory experimental equilibrium data are only rarely available for the particular conditions of temperature, pressure, and composition required in a particular design problem. It is therefore necessary to interpolate or extrapolate existing mixture data or, when suitable data are lacking, to estimate the desired equilibria from some appropriate correlation.

Activity coefficients may be measured experimentally or calculated theoretically, using the Debye Hückel equation or extensions such as Davies equation or specific ion interaction theory (SIT) may also be used. Alternatively correlative methods such as UNIQUAC, NRTL or UNIFAC may be employed, provided fitted component-specific or model parameters are available which are explained as below:

NON-RANDOM TWO LIQUID MODEL (NRTL)

The Non-Random Two Liquid model (NRTL model) is an activity coefficient model that correlates the activity coefficients γ_i of a compound i with its mole fractions x_i in the concerning liquid phase. It is frequently applied in the field of chemical engineering to calculate phase equilibria. The concept of NRTL is based on the hypothesis of Wilson that the local concentration around a molecule is different from the bulk concentration. This difference is due to a difference between the interaction energy of the central molecule with the molecules of its own kind and that with the molecules of the other kind. The energy difference introduces also non-randomness at the local molecular level. The NRTL model belongs to the so-called local composition models [Renon, Prausnitz 1968].

UNIQUAC MODEL

UNIQUAC (Universal Quasi Chemical) is an activity coefficient model used in description of phase equilibria [Abrams Prausnitz 1975]. The model is a so-called lattice model and has been derived from a first order approximation of interacting molecule surfaces in statistical thermodynamics. The model is however not fully thermodynamically consistent due to its two liquid mixture approach. In this approach the local concentration around one central molecule is assumed to be independent from the local composition around another type of molecule.

It has been shown that while the local compositions are correlated, ignoring this correlation gives little effect on the correlation of activity coefficients [McDermott 1976]. Today the UNIQUAC model is frequently applied in the description of phase equilibria (i.e. liquid solid, liquid-liquid or liquid-vapour equilibrium). The UNIQUAC model also serves as the basis of the development of the group contribution method UNIFAC, where molecules are subdivided in atomic groups.

UNIFAC MODEL

The UNIFAC method is a semi-empirical system for the prediction of non-electrolyte activity estimation in non-ideal mixtures. UNIFAC uses the functional groups present on the molecules that make up the liquid mixture to calculate activity coefficients. By utilizing interactions for each of the functional groups present on the molecules, as well as some binary interaction coefficients, the activity of each of the solutions can be calculated.

The calculated activity coefficient can be used for steady state simulation of distillation column. But Aspen provides some inbuilt property models which can be used as per the requirement of the problem. Hence we don't need supplying the property methods from outside.

1.2 OBJECTIVE OF CONTROL

Control of distillation column refers to achieve the 3 major objectives:

- (1) Material-balance control.
- (2) Product quality control and
- (3) Satisfaction of constraints.

Feedback, feed forward, material balance control, decoupling and cascade control are some of traditional approaches to distillation control. Different methods of controlling the columns have been reported till now in the literature. A few examples are optimization-based PI/PID control for a binary distillation column via a genetic searching algorithm (GSA) [2], fuzzy-neural-net-based (FNN) inferential controller to control high purity distillation column [3], model based controller to control binary distillation column product purities [4], integrated control scheme to control ETBE reactive distillation column [5]. There is not that much Literature available for Aspen Dynamics control configuration.

In present work, steady state simulations are performed and then sensitivity analysis etc. is done for going more into the process conditions. After this steady state solution is being exported in the Aspen Dynamics by supplying the physical dimension information regarding the distillation column. Then the performance of PI controller of Aspen Dynamics for controlling the purity in the distillate is observed while separating a provided mixture.

1.3 CONTROL STRATEGIES

Here the purity of distillate has been controlled using two strategies as below:

- (1) Tray temperature control.
- (2) Composition control.

The tray temperature and composition controllers are basically a PI controller which is tuned by the Tyreus–Luyben method. The tray temperature controller uses temperature as process variable and reboiler heat input as a manipulated variable. Composition controller uses mole fraction of one of the component as the process variable and reboiler heat input as a manipulating variable. Cascade controller if used, uses both the temperature and composition controllers together, where the tray temperature controller is the secondary controller. The purity of distillate for both servo and regulatory type situation is also controlled

CHAPTER 2

SIMULATION AND CONTROL OF THE COLUMN

2. SIMULATION AND CONTROL OF THE COLUMN

2.1 PROBLEM STATEMENT

(a) Methyl cyclohexane and toluene, when mixed form a close-boiling mixture which is difficult to separate by simple binary distillation processes. Thus we go for phenol which extracts toluene and thus allowing relatively pure methyl cyclohexane to be obtained in the overhead. The purity of the recovered methyl cyclohexane depends on the phenol input flow rate.

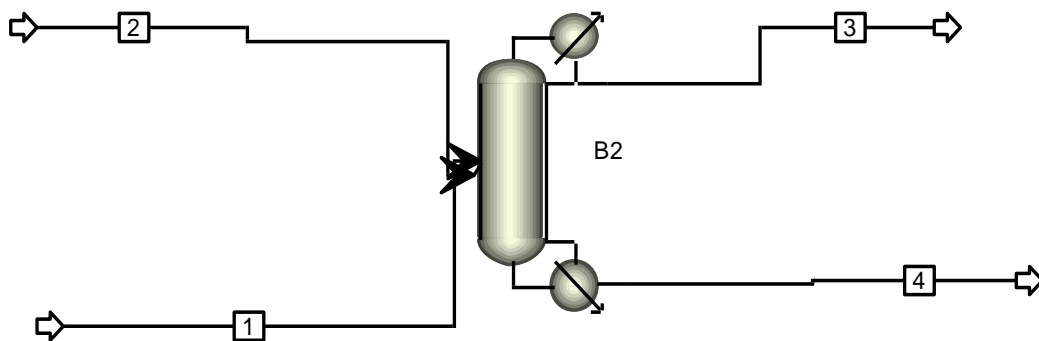


Fig. 1 Distillation Column

Table 1: Data table of the problem state 1

Serial No.	Name of The Chemical	Flow Rate(lbmol/hr)	Pressure (psia)	Temperature (F)
1.	Phenol	1200	20	220
2.	Methyl-Cyclo-Hexane	200	20	220
3.	Toluene	200	20	220

No. of equilibrium stages: 22

Total condenser is being used with a reflux ratio of 8. Further condenser and reboiler pressures are given as 16 psia and 20.2 psia respectively.

(b) A binary mixture of propane (0.4mole/mole) and iso-butane (0.6mole/mole) is to be separated in a tray tower distillation column containing 32 plates including reboiler and condenser. The overhead product is aimed as at least 95mole percent propane. The feed is introduced at a rate of 1.0 kmol/sec with 20 atm pressure and 322 K. The objective is to control the composition in the distillate, stage temperature inside the column, level of the reboiler and reflux drum, pressure of the condenser, and flow rate of the feed for both the servo and regulatory control schemes.

2.2 STEADY STATE SIMULATION

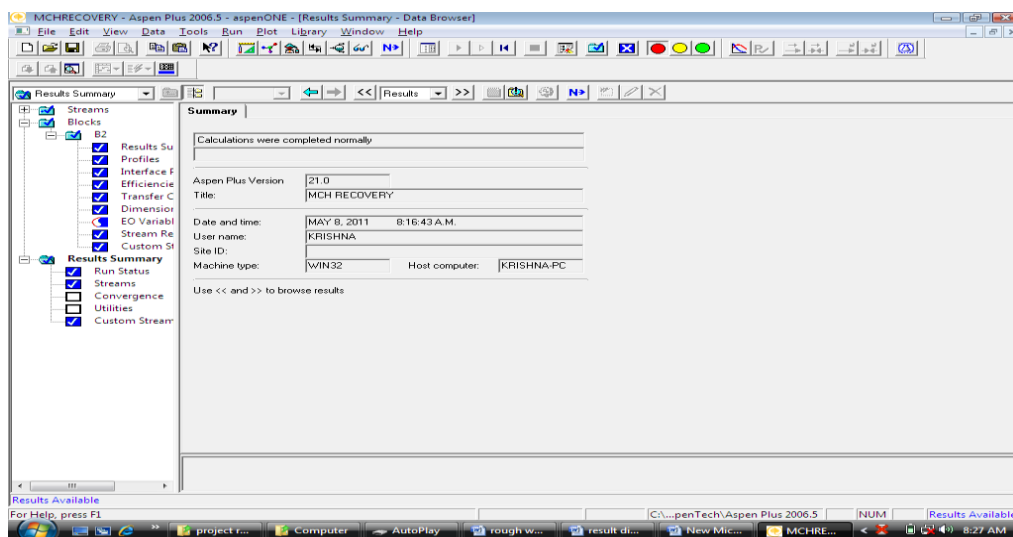


Fig. 2 Success Report Of Simulation

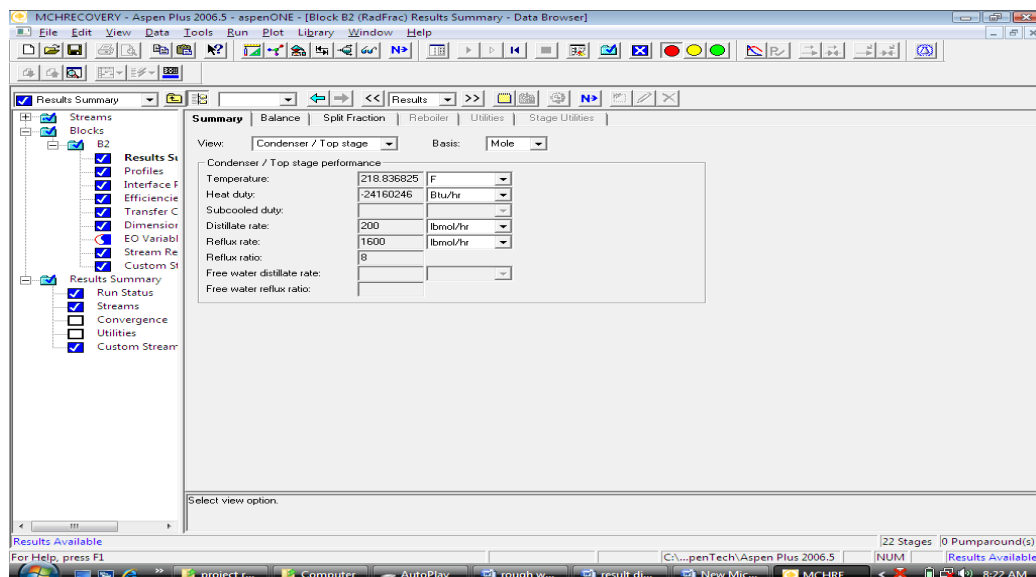


Fig.3 Block Results

Steady state simulations are performed for the given distillation column. And results obtained are presented in the form of tables directly from the simulated solutions.

Table 2: Stream Results

Material	Heat	Load	Work	Vol.% Curves	Wt. % Curves	Petro. Curves	Poly. Curves
Display: All streams Format: GEN_E Stream Table							
	1	2	3	4			
Temperature F	220.0	220.0	218.8	338.7			
Pressure psia	20.00	20.00	16.00	20.20			
Vapor Frac	0.000	0.000	0.000	0.000			
Mole Flow lbmol/hr	400.000	1800.000	200.000	2000.000			
Mass Flow lb/hr	38065.736	169403.472	19619.140	187850.068			
Volume Flow cuft/hr	827.177	2689.542	451.574	3291.139			
Enthalpy MMBtu/hr	-12.702	-107.917	-14.711	-93.888			
Mole Flow lbmol/hr							
TOLUENE	200.000		2.861	197.139			
PHENOL		1800.000	0.231	1798.709			
ETHYLCY	200.000		196.847	3.153			
Mole Frac							
TOLUENE	0.500		0.014	0.099			
PHENOL		1.000	0.001	0.900			
ETHYLCY	0.500		0.984	0.002			

Table 3: Variation of Flow Rate v/s Purity

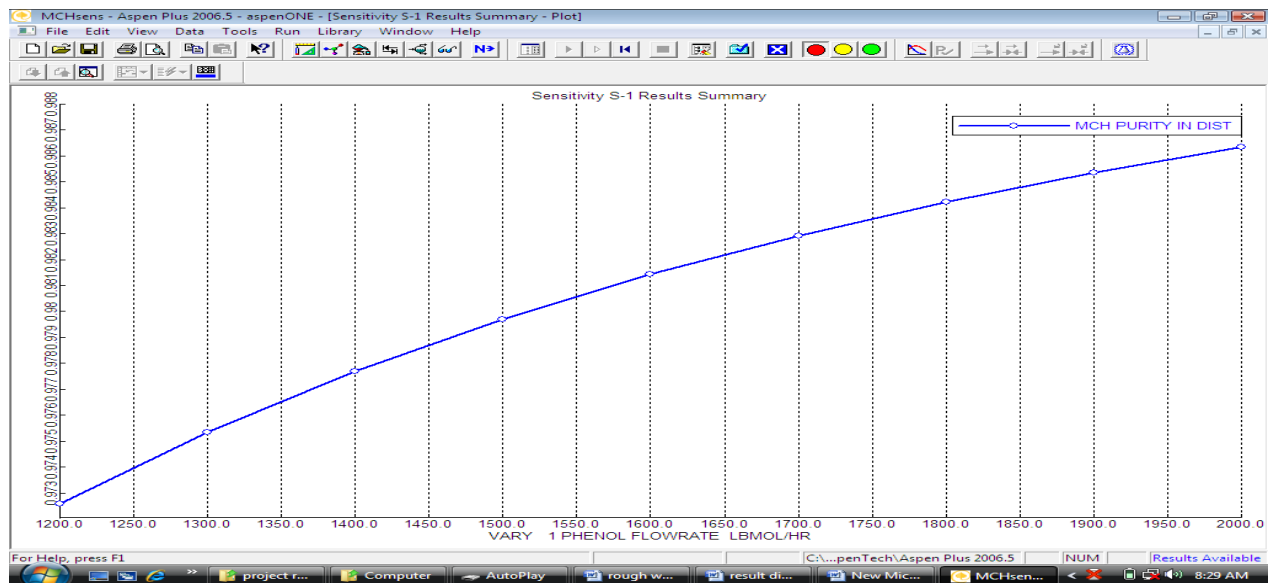
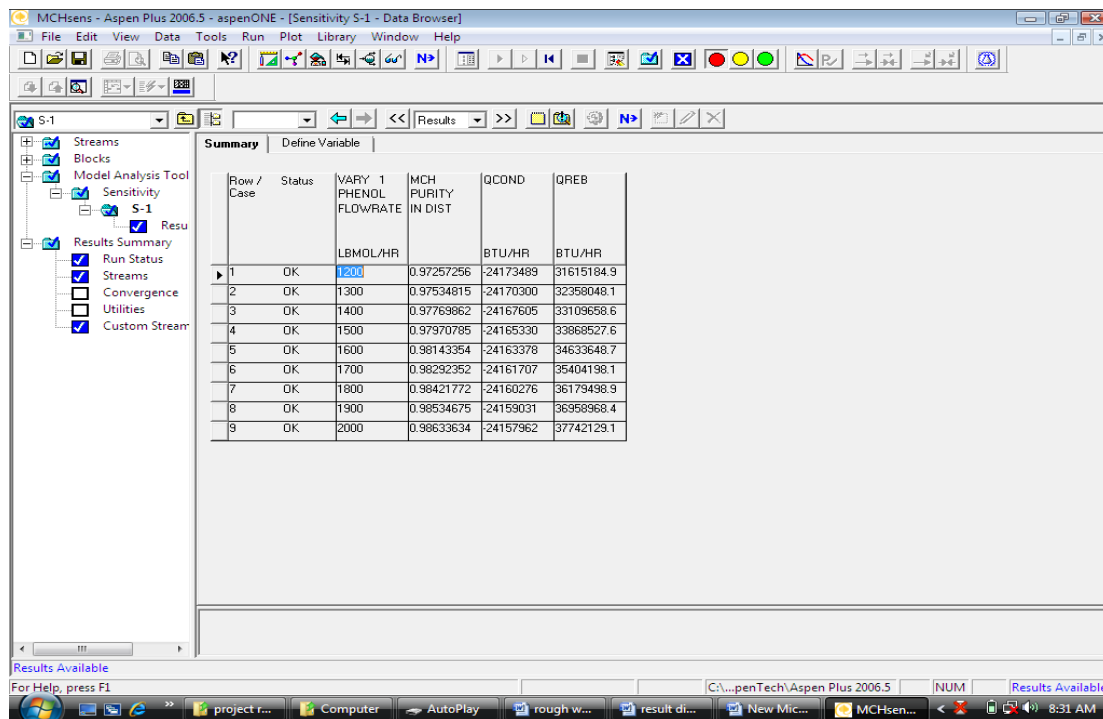


Fig. 4: Graph between flow rate vs purity

2.3 ASPEN DYNAMICS SIMULATION

After all the steady state simulations are being completed in the Aspen Plus, we get all the required results and perform necessary tabulation graphs which shows about the behaviour of system corresponding to the applied inputs. Then this information is exported into Aspen Dynamic. The Aspen Dynamics window appears accompanying default pressure controller (PC) with the closed loop process flow diagram. To get better operation of the column three additional controllers: Reflux drum level controller, Base-level controller and Feed flow controller are added.

After we are ready with the installation of the basic controllers on the column, the two strategies are being used for controlling distillate purity:

(1) Tray temperature controller.

(2) Composition controller.

In the simulation ideal PID controller [9] is used and it is given by

$$C = k + K_c \left\{ \varepsilon + \frac{1}{\tau_I} \int \varepsilon . dt + \tau_D \frac{d(\varepsilon)}{dt} \right\} \quad (1)$$

Where C is controller's output, k is the bias value, $\varepsilon = \text{Set Point} - \text{Process Variable}$, K_c , τ_I and τ_D are the controller's gains, integral time constant and derivative time constant respectively.

TRAY TEMPERATURE CONTROLLER

The tray temperature is maintained by tray temperature controller. It is connected with the tray which gives maximum gain for temperature change due to small change in the design variable. In this control action reflux ratio plays an important deciding factor.

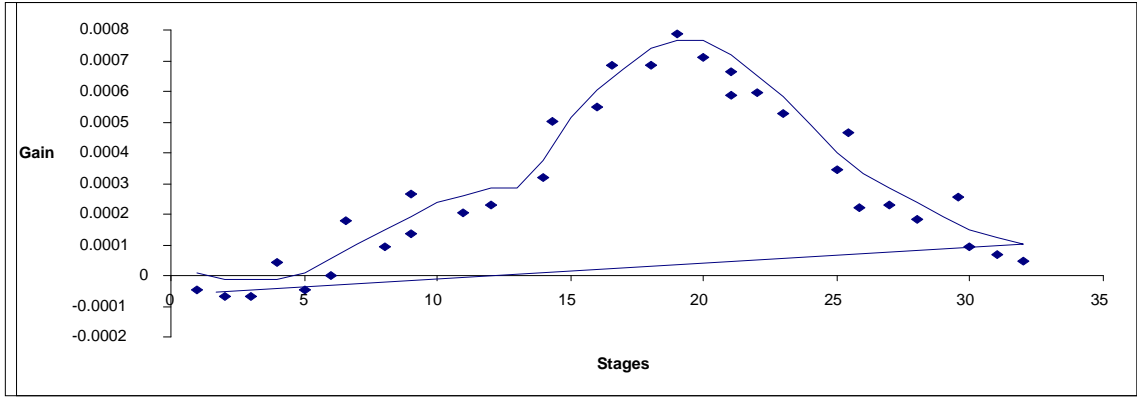


Fig. 5: Variation of steady state gain with tray for temperature controller

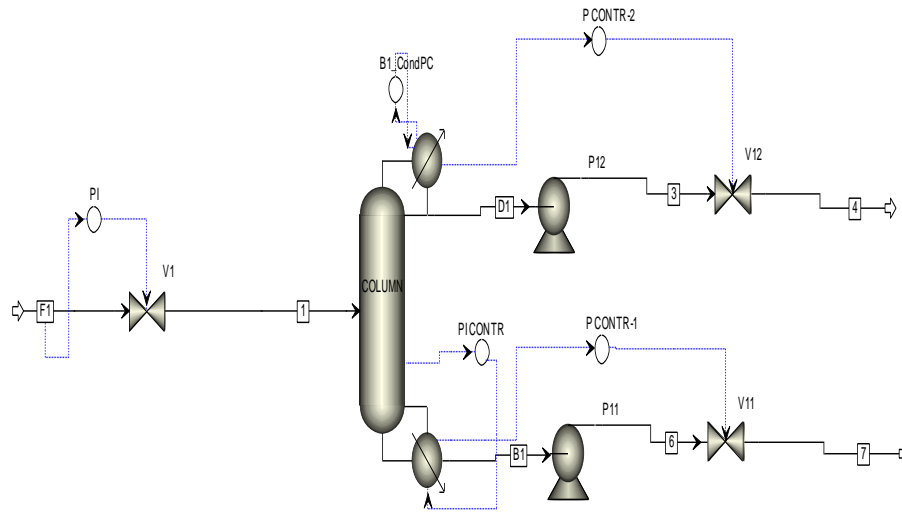


Fig. 6: Distillation column with tray temperature controller

As, Tyreus-Luyben provides more conservative settings and also more suitable for chemical process control applications [9], it is used to tune the tray temperature controller. The tuned parameters of the PI controller are controller gain, $K_c = 182.56$ and integral time constant,

$$\tau_i = 2.54 \text{ min.}$$

After installing and tuning the temperature controller, the performance of controller is tested for both servo and regulatory control scheme. In regulatory controlling scheme, the molar feed flow rate is increasing by 10% of its initial value. The performance of the regulatory controller at different set points is shown in Fig. 7. The figure illustrates how, new steady state purity

increases when we decrease the temperature. The required temperature to obtain 99 molar % distillate purity is 342.442K.

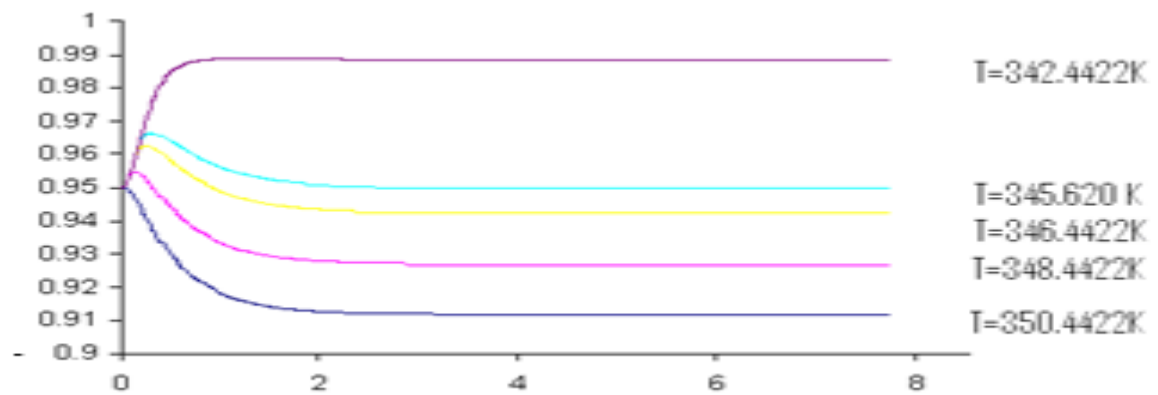


Fig. 7: Distillate purity versus time, when feed flow rate is increased by 10% of its initial value for differ temperature set points..

Furthermore targeting more than 99 percent molar purity of distillate, the controller is checked for servo controlling scheme. The performance of controller is shown in Fig. 10. It also shows that target purity can be achieved when the set point is 342.03 K.

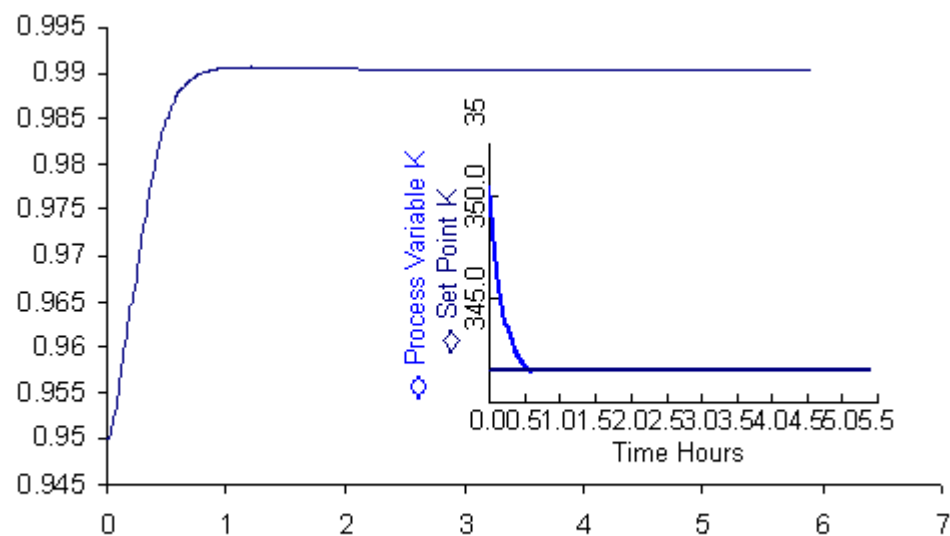


Fig. 8: Variation of temperature and purity when required distillate purity is set at 99 percent.

COMPOSITION CONTROLLER

Composition controller is a proportional integral controller which can give product purity at it desired level by manipulating the reboiler heat input.

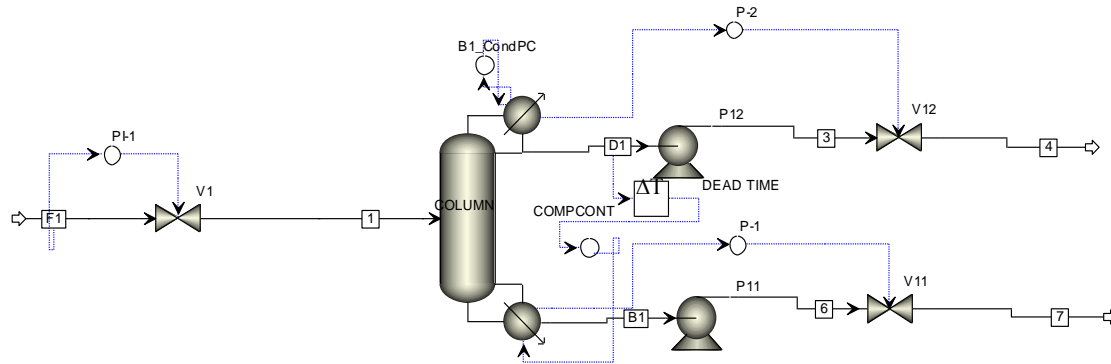


Figure 9: Distillation column with composition controller

After the tuning process, the controller is tested for servo and regulatory type problem. The tuned parameters of the controller are $K_C = 1.731$ and $\tau_I = 68.54$ min for the molar feed flow rate of 1.0 kmol/sec. In servo control scheme, the controller is tested for targeted value of 99% of purity in distillate. The controller performance is shown in Fig 12 which shows that it achieves the targeted value after 5.938 hr.

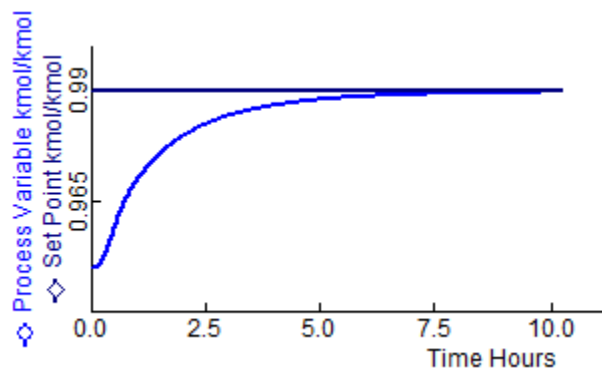


Figure 10: Variation of the purity of the distillate for the composition controller when 99 molar percent of purity in the distillate is set

After performing servo test for controller, the controller is tested for regulatory control scheme by changing the feed flow rate by 10% from its initial value (1kmol/sec).The performance of

controller is shown in Fig. 7 which indicates that after 6.65 hrs, the increased load have been removed and the controller reached the new steady state value (0.95 mole fraction of distillate)

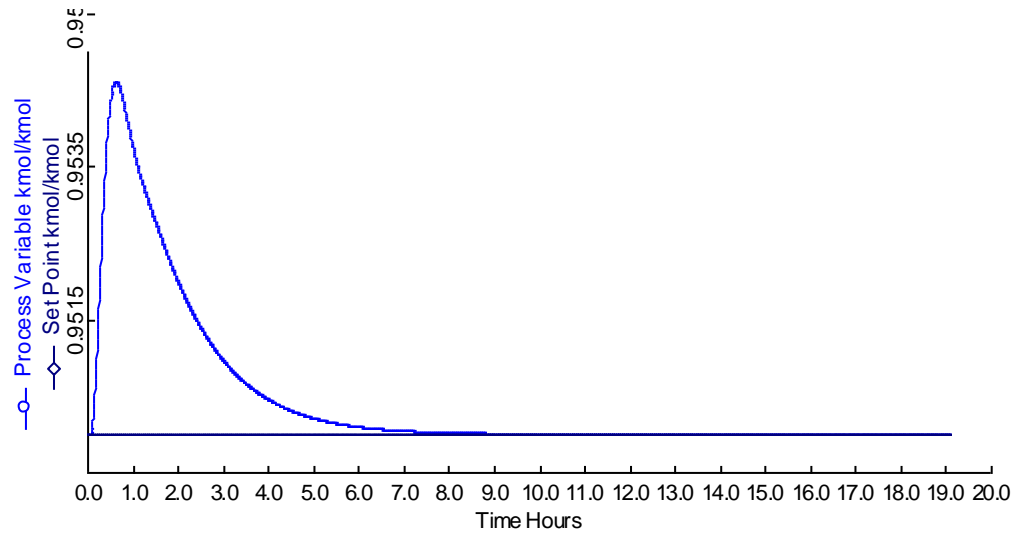


Fig. 11: Distillate purity for the composition controller when molar feed flow rate is increased by 10% of its initial value.

CHAPTER 3

RESULTS AND DISCUSSION

3. RESULTS AND DISCUSSION

After the successful completion of simulation, block and stream results are being presented in the Fig.3 and 4 respectively. Then we varied the flow rate of Phenol in the column. Now as we know that Phenol flow rate has an appreciable effect in the distillate purity, so the resulting information is being plotted in the form of a graph in the Fig. (6), it is clear from the Fig. (6), that Purity of Distillate is decided by the flow rate of Phenol. But as we know that, with the increase in flow rate; reboiler duty increases but condenser duty decreases. Hence an optimum value of feed rate of Phenol is to be decided in distillation columns to achieve a desired level of purity.

After tuning the temperature controller, tuning parameters are obtained as:

Controller gain, $K_c=182.56$ and integral time constant, $\tau_i=2.54\text{min}$.

Then the performance of temperature controller is tested for both servo and regulatory control scheme. In regulatory controlling scheme, the molar feed flow rate is increased by 10% of its initial value. The performance of the regulatory controller at different set points is shown in Fig. 9. The figure illustrates that, how new steady state purity increases when we decrease the temperature. The required temperature to obtain 99 molar % purity of distillate is 342.442K. The performance of servo controller is shown in Fig. 10. It also shows that target purity can be achieved when the set point is 342.03 K

Similarly for Composition controller, tuned parameters are given as:

Controller gain, $K_c=1.731$ and integral time constant, $\tau_i=68.54\text{min}$.

In regulatory control scheme, the performance of controller is shown in Fig. 7 which indicates that after 6.65 hours, the increased load have been removed and the controller reached the new steady state value (0.95 mole fraction of distillate)

While in servo control scheme, the controller is tested for targeted value of 99% distillate purity. The controller performance is shown in Fig 12 which shows that it achieves the targeted value after 5.938 hr.

Further observations show here that, Temperature control is fast controller (ultimate value 0.56 hr). While Composition control has shown slower response (ultimate value 5.938 hr in case of servo and 6.65 in case of regulatory).

CHAPTER 4

CONCLUSION AND SCOPE FOR FUTURE WORK

4. CONCLUSION AND SCOPE FOR FUTURE WORKS

Thus we see that Aspen makes it easy to build and run the process simulation model by providing with a comprehensive system of the online process modeling. Also Process simulation allows one to predict the behavior of a process by using basic engineering relationships, such as mass and energy balances, and phase and chemical equilibrium. From the obtained results, we observe that with simulation; one can design better plants and increase the profitability in the existing plants. Process simulation is helpful throughout the entire life of a process, from research and development through process design to production. Aspen Dynamics help in getting information about the behavior of installed control configuration. After tuning of the controller, we checked the behavior of controllers in regulatory as well as servo control schemes. On observing the respective responses, we see that temperature control has a faster response than the composition controller. Hence we can conclude that Aspen Dynamics helps in finding out the sensitivity of the controllers. In future; if it is properly interfaced with MATLAB, then it provides facility to control the more rigorous columns like reactive distillation columns etc.

CHAPTER 5

REFERENCES

5. REFERENCES

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